

Biphenyl

92-52-4 | DTXSID4020161

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2430 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.69e-01

Confidence level: 7.31e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Biphenyl</div> <div>Measured: 1860</div> <div>Predicted: 2430</div>	<div>Image not found</div> <div>2-Ethyl-naphthalene</div> <div>Measured: 5750</div> <div>Predicted: 3850</div>	<div>Image not found</div> <div>1-Ethyl-naphthalene</div> <div>Measured: 6030</div> <div>Predicted: 4360</div>
<div>Image not found</div> <div>Diphenyl oxide</div> <div>Measured: 1950</div> <div>Predicted: 1170</div>	<div>Image not found</div> <div>Safrole</div> <div>Measured: 676</div> <div>Predicted: 79.7</div>	